

**Discussion.** Final atomic parameters and equivalent isotropic temperature factors are given in Table 1.\* Numbering scheme, bond distances and intra-annular torsion angles are depicted in Fig. 1; bond angles are shown in Table 2.

Bond distances and angles are normal for this kind of molecule. In the *A* ring there is electron delocalization along the  $\Delta^{1-3,10}$ -dioxo system; bond distances around the spiro center C5 are slightly longer than normal (Birnbau & Ferguson, 1969). The *A* ring has a flattened half-chair conformation due to the  $\Delta^{1-3,10}$ -dioxo system. Rotational symmetry is dominant ( $\Delta C_2^{1-2} = 3.0$ ). The average of the intra-annular torsion angles is  $23.9^\circ$ . The five-membered *B* ring exhibits an  $8\beta$ -envelope conformation ( $\Delta C_2^5 = 1.9$ ). The *C* ring has a highly symmetrical chair conformation; all asymmetry parameters are below 4.6. The *D*-ring conformation is a  $14\alpha$  envelope ( $\Delta C_5^{14} = 1.3$ ). All ring junctions are *trans* as indicated by the relevant torsion angles. The configuration at C5 is *S*, deduced by comparison with other known chiral centers in the molecule; this is in agreement with chemical considerations of the reaction mechanism (Planas, Tomas & Bonet, 1987). Fig. 2 is a perspective view of the molecule and Fig. 3 is a monoscopic drawing of the molecular packing.

\* Lists of structure amplitudes, anisotropic thermal parameters, and complete molecular geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44608 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The authors are indebted to Professor J. J. Bonet (Instituto Químico de Sarrià, Barcelona, Spain) for suggesting the problem and providing the sample. We also would like to thank the 'Servei de Raigs-x del CSIC i la Generalitat de Catalunya' for the use of facilities enabling us to carry out the collection of X-ray diffraction data.

#### References

- BIERI, J. H., PREWO, R., BRIANSÓ, J. L. & PINIELLA, J. F. (1985). *Acta Cryst.* C41, 1530–1532.
- BIRNBAUM, K. B. & FERGUSON, G. (1969). *Acta Cryst.* B25, 720–730.
- DECLERCQ, J.-P., GERMAIN, G., WRIGHT, H. & WOOLFSON, M. M. (1980). YZARC80. A random approach to crystal structure determination. Univ. of Louvain, Belgium, and York, England.
- GAETE, W. (1985). ESTER. Program for crystal structure representation. Univ. Autònoma de Barcelona, Spain.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
- MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. Univ. of York, England, and Louvain, Belgium.
- PINIELLA, J. F. (1985). PhD Thesis. Departament de Cristal·lografia, Univ. Autònoma de Barcelona, Spain.
- PLANAS, A., TOMAS, J. & BONET, J. J. (1987). *Tetrahedron Lett.* 28, 471–474.
- RIUS, J. & MIRAVITLLES, C. (1987). ROTSEARCH87. A Patterson search program for X-ray crystal structure determination. Inst. Ciència de Materials, CSIC, Barcelona, Spain.
- SHELDRICK, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.

*Acta Cryst.* (1988). C44, 701–704

## Structure of Triphenylphosphine–Cyanoborane

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(Received 16 June 1987; accepted 18 November 1987)

**Abstract.**  $[P(C_6H_5)_3].BH_2CN$ ,  $M_r = 301.0$ , monoclinic,  $P2_1/n$  (from Weissenberg photograph and single-crystal diffractometry),  $a = 18.445$  (3),  $b = 9.554$  (2),  $c = 18.782$  (2) Å,  $\beta = 93.35$  (1)°,  $V = 3304.2$  (9) Å<sup>3</sup>,  $Z = 8$  (two formula units),  $D_m = 1.206$  (aq. KI),  $D_x = 1.210$  Mg m<sup>-3</sup>,  $\lambda(Mo K\alpha) = 0.71073$  Å,

$\mu = 16.5$  mm<sup>-1</sup>,  $F(000) = 1264$ , room temperature (293 K), final  $R = 0.044$  and  $wR = 0.057$  for 2623 observed reflections. The molecules have a tetrahedral overall structure and are held in the crystal by van der Waals forces only. The P–B bond distances in the two independent molecules differ slightly. The B–C≡N moiety is slightly non-linear.

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**Introduction.** Various derivatives of amine–boranes, in particular the cyano derivatives,  $(CH_3)_3N.BH_2CN$ ,

(CH<sub>3</sub>)<sub>2</sub>NH.BH<sub>2</sub>CN (Hall, Starnes, Spielvogel, Wisian-Nielson, Das & Wojnowich, 1979); O(CH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>-N(CH<sub>3</sub>)<sub>2</sub>.BH<sub>2</sub>CN and NCCH<sub>2</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub>.BH<sub>2</sub>CN (Hall, Gilbert, McPhail, Morse, Hassett & Spielvogel, 1985), which may be regarded as the precursors of boron analogues of  $\alpha$ -amino acids, have been shown to exhibit significant (80%) inhibition against Ehrlich Ascites carcinoma growth in CF<sub>1</sub> male-mice models. As phosphorus is an essential constituent of living organisms, it is expected that analogous phosphorus compounds may also have biological activity and hence one of us reported the synthesis of a few phosphine-cyanoboranes (Das & Roy, 1985, 1986). Since no X-ray structural study on amine-cyanoboranes except ammonia-cyanoborane and phosphine-cyanoborane has been reported so far, we have solved the structure of a phosphine-cyanoborane to obtain structural information useful for understanding the activity of this class of compounds.

**Experimental.** Colourless crystals (0.47 × 0.35 × 0.28 mm) of the title compound obtained from an ethanolic solution of the compound by slow evaporation at room temperature. Data taken on an Enraf-Nonius CAD-4 diffractometer, graphite-monochromatized Mo K $\alpha$  radiation. Cell dimensions refined by 25 accurately centred reflections in range 22 < 2 $\theta$  < 37°. Orientation controlled after every 200 reflections. Intensity checked by three standard reflections (21 $\bar{3}$ , 211 and 60 $\bar{6}$ ) after each 3600 s exposure, no significant variation of intensity observed;  $\theta$  range 0–25° (intensities negligible at  $\theta$  > 25°), ranges of  $h, k, l$  0–22, 0–11, –22–22. Out of 6300 reflections, 2627 reflections had intensities less than 4 $\sigma$ ( $F_o$ ) and were classed as unobserved. Lp correction applied, absorption ignored. Reflections 204, 20 $\bar{4}$ , 402 and 40 $\bar{4}$  were affected greatly by extinction and were subsequently eliminated from final refinement list.

Structure solved by direct methods (*MULTAN78*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *E*-map model gave  $R = 0.392$ . Positional and anisotropic thermal parameters of 44 non-H atoms were refined by block-diagonal least squares to  $R = 0.091$  and  $wR = 0.112$ . The positions of 30 H atoms (linked with phenyl rings) out of 34 H atoms were calculated from known geometry around C atoms (bond distance fixed at 1.08 Å). Four H atoms (H1B, H2B, H3B, H4B) associated with the two B atoms were found from  $\Delta F$  synthesis. The H atoms were assigned temperature factors of the atoms to which they are covalently attached. The anisotropic refinement of 44 non-H atoms and isotropic refinement of 34 H atoms (532 parameters) gave  $R = 0.060$ ,  $wR = 0.081$ .  $w(\Delta F)^2$  minimized with weighting factor  $w = 1/\sigma^2(F)$ , where  $\sigma(F) = R_i |F_o|$  (Seal & Ray, 1981) where  $R_i = \sum(|F_o| - |F_c|) / \sum |F_o|$  and  $i$  stands for different ranges of  $F_o$  values divided into segments of equal

numbers in order of increasing values. Final  $R = 0.044$  and  $wR = 0.057$ ;  $\Delta F$  map featureless (max., min. heights  $\pm 0.20 e \text{ \AA}^{-3}$ ),  $S$ (goodness of fit) = 1.32,  $(\Delta/\sigma)_{\text{max}} = 0.336$  and  $(\Delta/\sigma)_{\text{av}} = 0.127$  for non-H atoms. Scattering factors for C, N, B and P atoms from Cromer & Liberman (1970) and for H atoms from Stewart, Davidson & Simpson (1965); Burroughs 6700 computer (Regional Computer Centre, Calcutta); modified versions of *MAMIE* and *BLOK* from the *XRAY ARC* program system (Vickery, Bright & Mallinson, 1973).

**Discussion.** The molecular packing as viewed down the  $b$  axis is shown in Fig. 1. The atomic coordinates are listed in Table 1 and interatomic distances and angles in Table 2.\* One of the three P–C bond distances varies significantly from the other two. A comparison of the data with those of triphenylphosphine itself or a comparison with P–C single-bond distances calculated from covalent radii (Sutton, 1958, 1965) would help to explain this finding. The shortening of one P–C bond distance may be due to differences in the  $\pi$  bonding of the three phenyl rings (depending on the orientations of the rings with respect to the P  $d$   $\pi$  orbitals). The P–B bond distances in the two molecules also differ slightly [P1–B1 = 1.996 (6), P2–B2 = 1.917 (7) Å]. The bond angles at P are somewhat distorted but not significantly enough to warrant major discussion. The average B–CN bond distance, 1.57 Å in this com-

\* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44558 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

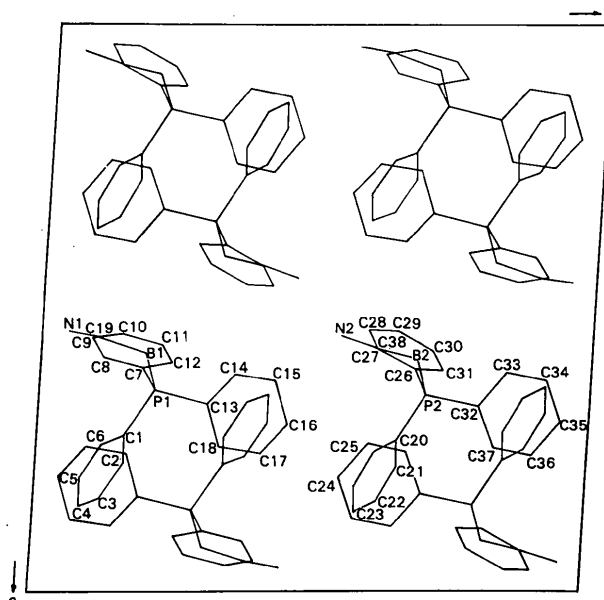


Fig. 1. Projection of the structure down the  $b$  axis.

Table 1. Atomic coordinates ( $\times 10^4$ ) and isotropic temperature factors ( $\text{\AA}^2$ )
$$B_{\text{eq}} = \frac{4}{3} \sum_i \sum_j \beta_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	$B_{\text{eq}}$
P1	2102 (1)	3339 (1)	6439 (1)	2.9
B1	1889 (3)	1772 (7)	5781 (3)	4.4
C19	1052 (3)	1780 (5)	5570 (3)	4.5
N1	439 (3)	1763 (6)	5418 (3)	7.1
C1	3068 (2)	3297 (5)	6682 (2)	3.1
C2	3548 (3)	3260 (6)	6155 (3)	4.2
C3	4283 (3)	3165 (7)	6297 (3)	5.1
C4	4550 (3)	3097 (6)	7014 (3)	4.9
C5	4084 (3)	3127 (6)	7545 (3)	4.7
C6	3334 (3)	3230 (5)	7397 (2)	3.7
C7	1612 (2)	3254 (5)	7239 (2)	3.1
C8	1214 (3)	2068 (5)	7398 (2)	3.7
C9	826 (3)	2020 (6)	7999 (3)	4.6
C10	832 (3)	3153 (7)	8458 (3)	4.8
C11	1132 (3)	4331 (6)	8316 (3)	4.8
C12	1615 (3)	4388 (5)	7712 (3)	4.1
C13	1890 (2)	5055 (5)	6062 (2)	2.9
C14	1168 (3)	5326 (5)	5860 (3)	3.9
C15	968 (3)	6623 (6)	5573 (3)	4.7
C16	1498 (4)	7641 (6)	5494 (3)	5.3
C17	2213 (3)	7377 (5)	5698 (3)	3.6
C18	2410 (3)	6085 (5)	5981 (2)	3.9
P2	7028 (1)	4469 (1)	6515 (1)	2.8
B2	6840 (3)	6093 (7)	5935 (3)	4.2
C38	6016 (3)	6334 (6)	5709 (3)	4.6
N2	5424 (3)	6556 (6)	5540 (3)	6.6
C20	6815 (2)	2815 (4)	6078 (2)	2.9
C21	7288 (3)	1686 (5)	6096 (2)	3.8
C22	7092 (3)	435 (5)	5771 (3)	4.4
C23	6419 (3)	290 (5)	5425 (3)	4.7
C24	5943 (3)	1400 (6)	5403 (3)	4.5
C25	6128 (3)	2669 (5)	5712 (3)	4.0
C26	6565 (2)	4476 (5)	7335 (2)	3.0
C27	6159 (3)	5640 (5)	7519 (2)	2.4
C28	5796 (3)	5663 (6)	8139 (3)	4.1
C29	5840 (3)	4513 (6)	8603 (3)	4.4
C30	6243 (3)	3370 (6)	8417 (3)	4.7
C31	6593 (3)	3329 (5)	7793 (3)	3.7
C32	7994 (2)	4456 (5)	6720 (2)	3.2
C33	8294 (3)	4487 (5)	7439 (3)	3.7
C34	9035 (3)	4564 (6)	7565 (3)	4.5
C35	9488 (3)	4587 (6)	7024 (3)	5.0
C36	9204 (3)	4530 (6)	6313 (3)	4.9
C37	8457 (3)	4473 (6)	6175 (3)	4.1

Table 2. Bond distances ( $\text{\AA}$ ) and bond angles ( $^\circ$ ) (e.s.d.'s in parentheses)

P1-B1	1.996 (6)	P2-B2	1.917 (7)
B1-C19	1.571 (7)	B2-C38	1.571 (7)
C19-N1	1.150 (8)	C38-N2	1.139 (8)
P1-C1	1.813 (4)	P2-C20	1.813 (4)
P1-C7	1.800 (4)	P2-C26	1.804 (4)
P1-C13	1.819 (4)	P2-C32	1.800 (4)
C1-C2	1.366 (6)	C20-C21	1.386 (6)
C2-C3	1.369 (7)	C21-C22	1.380 (6)
C3-C4	1.408 (7)	C22-C23	1.374 (7)
C4-C5	1.354 (8)	C23-C24	1.376 (7)
C5-C6	1.398 (7)	C24-C25	1.378 (7)
C6-C1	1.404 (5)	C20-C25	1.412 (6)
C7-C8	1.392 (6)	C26-C27	1.395 (6)
C8-C9	1.372 (7)	C27-C28	1.377 (7)
C9-C10	1.383 (8)	C28-C29	1.401 (8)
C10-C11	1.289 (8)	C29-C30	1.377 (8)
C11-C12	1.483 (8)	C30-C31	1.371 (8)
C12-C7	1.401 (7)	C26-C31	1.392 (6)
C13-C14	1.387 (6)	C32-C33	1.429 (6)
C14-C15	1.392 (7)	C33-C34	1.375 (7)
C15-C16	1.393 (8)	C34-C35	1.353 (8)
C16-C17	1.375 (9)	C35-C36	1.406 (7)
C17-C18	1.384 (6)	C36-C37	1.388 (7)
C18-C13	1.388 (6)	C32-C37	1.371 (7)
C1-P1-C7	108.8 (2)	C20-P2-C26	106.8 (2)
C1-P1-C13	107.6 (2)	C32-P2-C26	109.2 (2)
P1-B1-C19	108.2 (4)	P2-B2-C38	114.3 (4)
B1-C19-N1	178.8 (5)	B2-C38-N2	177.6 (6)
C1-C2-C3	122.4 (5)	C20-C21-C22	120.9 (4)
C2-C3-C4	118.4 (5)	C21-C22-C23	120.1 (4)
C3-C4-C5	120.1 (5)	C22-C23-C24	119.6 (5)
C4-C5-C6	121.2 (5)	C23-C24-C25	121.5 (5)
C5-C6-C1	118.6 (4)	C24-C25-C20	119.0 (5)
C6-C1-C2	119.1 (4)	C25-C20-C21	118.7 (4)
C7-C8-C9	120.7 (4)	C26-C27-C28	121.1 (4)
C8-C9-C10	120.0 (5)	C27-C28-C29	119.9 (5)
C9-C10-C11	122.8 (5)	C28-C29-C30	118.4 (5)
C10-C11-C12	118.3 (5)	C29-C30-C31	121.8 (5)
C11-C12-C7	118.4 (4)	C30-C31-C26	120.2 (4)
C12-C7-C8	118.4 (4)	C31-C26-C27	118.3 (4)
C13-C14-C15	120.0 (5)	C32-C33-C34	119.3 (5)
C14-C15-C16	119.4 (5)	C33-C34-C35	121.5 (5)
C15-C16-C17	120.6 (5)	C34-C35-C36	120.0 (5)
C16-C17-C18	119.7 (5)	C35-C36-C37	119.3 (5)
C17-C18-C13	120.4 (5)	C36-C37-C32	121.0 (5)
C18-C13-C14	119.7 (4)	C37-C32-C33	118.7 (4)

compound, compares favourably with 1.56  $\text{\AA}$  found in  $(\text{BH}_2\text{CN})_6$  (McPhail & McFadden, 1975), 1.589  $\text{\AA}$  in  $\text{H}_3\text{N.BH}_2\text{CN}$  (McPhail, Onan, Spielvogel & Wisian-Neilson, 1978) and 1.577  $\text{\AA}$  in  $[\text{Na}(\text{H}_3\text{N.BH}_2\text{CN})_6]\text{I}$  (Hargrave, McPhail, Spielvogel & Wisian-Neilson, 1977). These literature values are close to the expected value and also to that found in  $\text{B}(\text{CH}_3)_3$  (Muetterties, 1967).

The C-N distances [1.150 (8), 1.139 (8)  $\text{\AA}$ ] are quite close to  $\text{C}\equiv\text{N}$  distances of 1.14  $\text{\AA}$  in  $(\text{BH}_2\text{CN})_6$ , 1.141  $\text{\AA}$  in  $\text{H}_3\text{N.BH}_2\text{CN}$  and 1.152  $\text{\AA}$  in  $[\text{Na}(\text{H}_3\text{N.BH}_2\text{CN})_6]\text{I}$ , and all other simple  $\text{C}\equiv\text{N}$ -containing molecules such as  $(\text{CN})_2$ ,  $\text{HCN}$ ,  $\text{RCN}$  ( $R = \text{alkyl}$ ),  $\text{XCN}$  ( $X = \text{halogen}$ ) and  $\text{CN}^-$  (range 1.15–1.167  $\text{\AA}$ ; Greenwood & Earnshaw, 1984). The valency angles subtended at the B atoms, P-B-C, having values of 108.2 (4) and 114.3 (4) $^\circ$ , are either in agreement or a little high compared with the ideal tetrahedral angle of 109 $^\circ$  28'. The B-C $\equiv$ N moiety is slightly non-linear, which is not unusual and is in conformity with 179.6 $^\circ$  found in  $\text{H}_3\text{N.BH}_2\text{CN}$  and 175.8 $^\circ$  in  $[\text{Na}(\text{H}_3\text{N.BH}_2\text{CN})_6]\text{I}$ .

The authors thank the Geological Survey of India (Calcutta) for helping them in taking the intensity data. Computational work was carried out at the Regional Computer Centre, Calcutta. MKD thanks DST, Government of India, for financial assistance.

#### References

- CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.
- DAS, M. K. & ROY, S. (1985). *Synth. React. Inorg. Met. Org. Chem.* **15**, 53–59.
- DAS, M. K. & ROY, S. (1986). *Synth. React. Inorg. Met. Org. Chem.* **16**, 67–75.
- GREENWOOD, N. N. & EARNSHAW, A. (1984). *Chemistry of the Elements*, p. 337. Oxford: Pergamon Press.
- HALL, I. H., GILBERT, C. J., MCPHAIL, A. T., MORSE, K. W., HASSETT, K. & SPIELVOGEL, B. F. (1985). *J. Pharm. Sci.* **74**, 755–758.
- HALL, I. H., STARNES, C. O., SPIELVOGEL, B. F., WISIAN-NEILSON, P., DAS, M. K. & WOJNOWICH, L. (1979). *J. Pharm. Sci.* **68**, 685–688.
- HARGRAVE, K. D., MCPHAIL, A. T., SPIELVOGEL, B. F. & WISIAN-NEILSON, P. (1977). *J. Chem. Soc. Dalton Trans.* pp. 2150–2153.

- MCPhAIL, A. T. & MCFADDEN, D. L. (1975). *J. Chem. Soc. Dalton Trans.* pp. 1784–1786.
- MCPhAIL, A. T., ONAN, K. D., SPIELVOGEL, B. F. & WISIAN-NEILSON, P. (1978). *J. Chem. Res. (S)*, pp. 205–208.
- MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.
- MUETTERTIES, E. L. (1967). *The Chemistry of Boron and its Compounds*, p. 514. New York: John Wiley.
- SEAL, A. & RAY, S. (1981). *Indian J. Phys.* 55A, 414–416.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* 42, 3175–3187.
- SUTTON, L. E. (1958). *Tables of Interatomic Distances and Configuration in Molecules and Ions*. Spec. Publ. No. 11. London: The Chemical Society.
- SUTTON, L. E. (1965). *Tables of Interatomic Distances and Configuration in Molecules and Ions. Supplement*. Spec. Publ. No. 18. London: The Chemical Society.
- VICKERY, B. L., BRIGHT, D. & MALLINSON, P. R. (1973). *XRAY ARC*. IBM1130 program system for crystallography modified for the Burroughs B6700 computer. Agricultural Research Council, London, England.

*Acta Cryst.* (1988). C44, 704–706

## Structure of 2,2,4,6-Tetraphenyldihydro-1,3,5-triazine Ethanol Solvate

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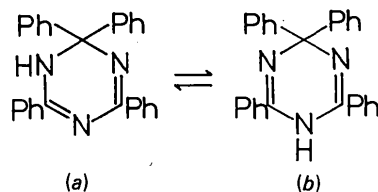
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(Received 26 October 1987; accepted 18 December 1987)

**Abstract.**  $C_{27}H_{21}N_3 \cdot C_2H_6O$ ,  $M_r = 433.5$ , monoclinic,  $P2_1/a$ ,  $a = 16.670$  (1),  $b = 13.5270$  (8),  $c = 10.7697$  (7) Å,  $\beta = 100.520$  (8)°,  $V = 2387.7$  (3) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.206$  g cm<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.54184$  Å,  $\mu = 5.03$  cm<sup>-1</sup>,  $F(000) = 920$ ,  $T = 293$  K,  $R = 0.071$  for 3322 observed reflections. 2,2,4,6-Tetraphenyldihydro-1,3,5-triazine exists in the 2,3-dihydro form, one of the two possible tautomers. The triazine and ethanol molecules are connected alternately by N(3)–H...O and N(5)...H–O hydrogen bonds to form a ribbon along the  $b$  axis, which seems to be responsible for the fact that this inclusion compound does not show photocoloration, unlike the inclusion compounds composed of acetone or tetrahydrofuran.

**Introduction.** 2,2,4,6-Tetraphenyldihydro-1,3,5-triazine was reported to exhibit photochromism in the solid state (Lottermoser, 1896) but the structure of the colored species has not been determined. Previously, one of the authors reported that the triazine exists in an equilibrium mixture of 2,3-dihydro (*a*) and 2,5-dihydro (*b*) forms, which are prototropic tautomers, in solution and in the solid state (Maeda, Kihara & Ishimura, 1985). Recently we found that the triazine formed crystalline inclusion compounds with various solvent molecules with a molar ratio of 1:1 on recrystallization. For acetone, chloroform, and tetrahydrofuran the colorless inclusion compounds turned red on exposure to UV light and the red color faded gradually in the dark, while the inclusion compounds composed of ethanol or 2-propanol showed no color change even

under prolonged irradiation. In order to clarify a relationship between structure and photocoloration for both types of inclusion compound, we have determined the molecular and crystal structure of the title compound.



**Experimental.** The triazine was synthesized by the method of Lottermoser (1896). Colorless plate-like crystals from an ethanol solution; systematic absences:  $h0l$   $h = 2n + 1$ ,  $0k0$   $k = 2n + 1$ ; crystal dimensions  $0.3 \times 0.2 \times 0.5$  mm, sealed in a glass capillary, Rigaku AFC-4 diffractometer, graphite monochromator; cell parameters refined by least squares on the basis of 16 independent  $2\theta$  values, Cu  $K\alpha$  radiation ( $45 < 2\theta < 59^\circ$ ); intensity measurement performed up to  $2\theta = 125^\circ$  ( $h = -21$  to  $21$ ,  $k = 0$  to  $16$ ,  $l = 0$  to  $14$ );  $\omega$ - $2\theta$  scan technique, scan speed  $4^\circ \text{ min}^{-1}$  in  $\theta$ , scan width  $(1.0 + 0.15 \tan \theta)^\circ$ ; background 5 s before and after each scan; three standard reflections (460,  $\bar{9}21$ , 006) monitored every 50 reflections, no significant variation in intensities; 3823 reflections measured, 3322 with  $|F_o| > 3\sigma(|F_o|)$  considered as observed and used for structure determination; corrections for Lorentz and polarization effects, absorption ignored; direct methods (*MULTAN78*, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and subsequent difference

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